



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2022 – 08:08 PM JST

PDB ID : 7V98
Title : Crystal Structure of the Dimeric EcHsp60
Authors : Lai, M.C.; Lin, S.M.
Deposited on : 2021-08-24
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at <http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.30
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

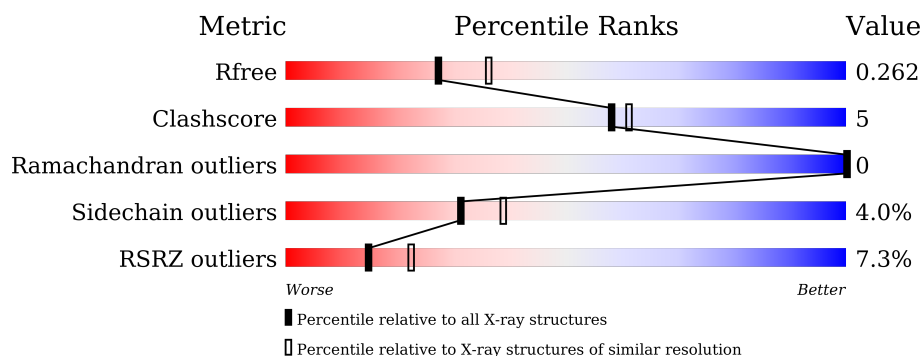
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	586	<div> <div>6%</div> <div>55%</div> <div>10%</div> <div>34%</div> </div>
1	B	586	<div> <div>4%</div> <div>56%</div> <div>10%</div> <div>34%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5796 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			2855	1788	499	559	9			
1	B	386	Total	C	N	O	S	0	0	0
			2860	1791	499	561	9			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	330	VAL	MET	engineered mutation	UNP A0A097BVP4
A	579	LEU	-	expression tag	UNP A0A097BVP4
A	580	GLU	-	expression tag	UNP A0A097BVP4
A	581	HIS	-	expression tag	UNP A0A097BVP4
A	582	HIS	-	expression tag	UNP A0A097BVP4
A	583	HIS	-	expression tag	UNP A0A097BVP4
A	584	HIS	-	expression tag	UNP A0A097BVP4
A	585	HIS	-	expression tag	UNP A0A097BVP4
A	586	HIS	-	expression tag	UNP A0A097BVP4
B	330	VAL	MET	engineered mutation	UNP A0A097BVP4
B	579	LEU	-	expression tag	UNP A0A097BVP4
B	580	GLU	-	expression tag	UNP A0A097BVP4
B	581	HIS	-	expression tag	UNP A0A097BVP4
B	582	HIS	-	expression tag	UNP A0A097BVP4
B	583	HIS	-	expression tag	UNP A0A097BVP4
B	584	HIS	-	expression tag	UNP A0A097BVP4
B	585	HIS	-	expression tag	UNP A0A097BVP4
B	586	HIS	-	expression tag	UNP A0A097BVP4

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	35	Total	O	0	0
			35	35		

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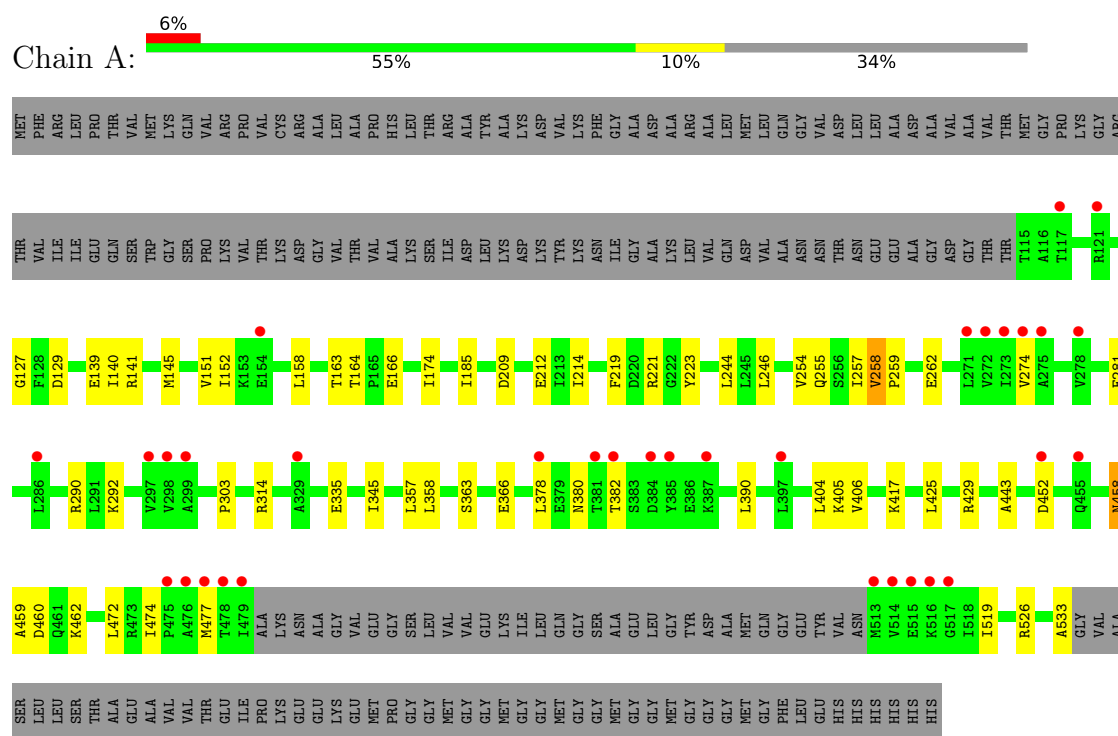
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	46	Total	O	0	0
			46	46		

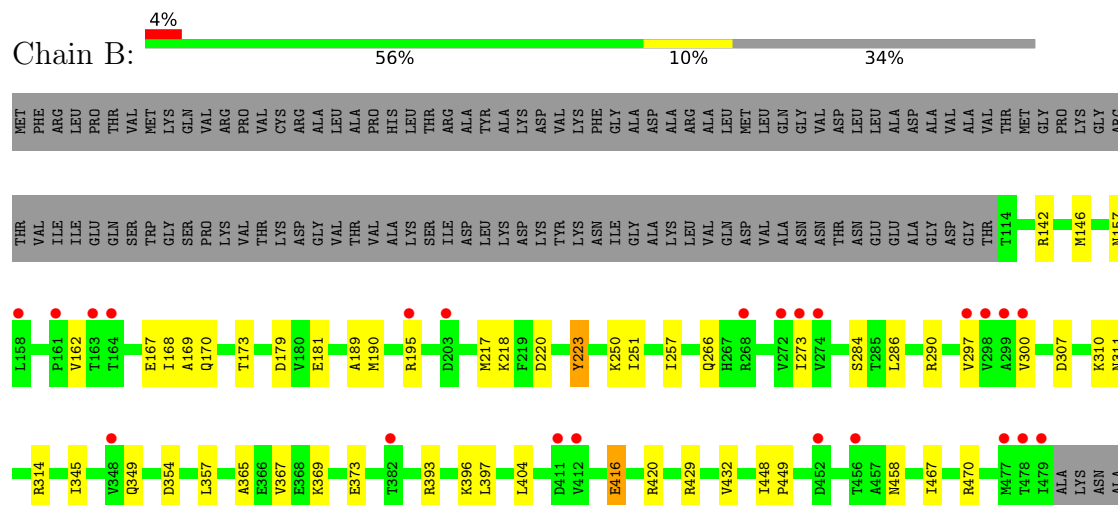
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 60 kDa chaperonin



- Molecule 1: 60 kDa chaperonin



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.29Å 95.38Å 128.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 2.35 29.96 – 2.35	Depositor EDS
% Data completeness (in resolution range)	91.5 (29.96-2.35) 86.1 (29.96-2.35)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.213 , 0.264 0.212 , 0.262	Depositor DCC
R_{free} test set	1972 reflections (4.65%)	wwPDB-VP
Wilson B-factor (Å ²)	46.1	Xtriage
Anisotropy	0.345	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5796	wwPDB-VP
Average B, all atoms (Å ²)	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.25	0/2879	0.47	0/3892
1	B	0.24	0/2884	0.46	0/3900
All	All	0.24	0/5763	0.47	0/7792

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2855	0	2946	29	0
1	B	2860	0	2955	29	0
2	A	35	0	0	0	0
2	B	46	0	0	3	0
All	All	5796	0	5901	56	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (56) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:GLU:OE2	1:A:405:LYS:NZ	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:LYS:NZ	2:B:603:HOH:O	2.33	0.61
1:B:345:ILE:HD13	1:B:357:LEU:HD22	1.84	0.60
1:A:127:GLY:HA2	1:B:467:ILE:HG12	1.82	0.59
1:B:514:VAL:HG22	1:B:519:ILE:HD11	1.83	0.59
1:A:174:ILE:HD12	1:A:519:ILE:HD11	1.84	0.59
1:B:167:GLU:HA	1:B:170:GLN:HG3	1.82	0.59
1:A:164:THR:HG22	1:A:166:GLU:H	1.67	0.58
1:B:367:VAL:HG13	1:B:397:LEU:HD22	1.84	0.58
1:B:257:ILE:HD11	1:B:273:ILE:HD13	1.84	0.58
1:B:169:ALA:O	1:B:173:THR:OG1	2.21	0.58
1:A:152:ILE:HG12	1:A:526:ARG:HG3	1.86	0.57
1:A:139:GLU:HB3	1:A:458:ASN:HD21	1.70	0.55
1:B:429:ARG:NH1	2:B:602:HOH:O	2.32	0.55
1:B:179:ASP:O	1:B:181:GLU:N	2.39	0.54
1:B:189:ALA:HB2	1:B:404:LEU:HD11	1.89	0.54
1:B:521:PRO:HB2	1:B:524:VAL:HG23	1.90	0.54
1:A:258:VAL:HG12	1:A:259:PRO:HD3	1.90	0.53
1:A:140:ILE:HG13	1:A:460:ASP:HB3	1.90	0.53
1:A:254:VAL:HG13	1:A:281:GLU:HG3	1.90	0.52
1:A:244:LEU:HB2	1:A:345:ILE:HD11	1.91	0.51
1:A:158:LEU:HD21	1:A:443:ALA:HB1	1.93	0.51
1:A:255:GLN:NE2	1:A:335:GLU:OE2	2.44	0.50
1:B:190:MET:HE3	1:B:195:ARG:HA	1.94	0.49
1:A:363:SER:OG	1:A:366:GLU:HG2	2.12	0.49
1:A:459:ALA:HA	1:A:462:LYS:HE3	1.95	0.49
1:A:129:ASP:OD1	1:B:470:ARG:NH2	2.47	0.48
1:B:218:LYS:HE2	1:B:354:ASP:HB3	1.95	0.48
1:B:416:GLU:OE2	1:B:420:ARG:NH1	2.45	0.48
1:A:345:ILE:HD13	1:A:357:LEU:HD22	1.96	0.47
1:A:425:LEU:O	1:A:429:ARG:HG3	2.15	0.47
1:B:349:GLN:NE2	2:B:608:HOH:O	2.48	0.47
1:A:164:THR:HG22	1:A:166:GLU:N	2.30	0.47
1:B:307:ASP:HA	1:B:310:LYS:HD2	1.97	0.47
1:B:190:MET:HE1	1:B:432:VAL:HG11	1.97	0.46
1:A:214:ILE:HD11	1:A:358:LEU:HD13	1.97	0.46
1:A:219:PHE:CD1	1:A:303:PRO:HG3	2.52	0.45
1:A:378:LEU:HD13	1:A:390:LEU:HB2	1.97	0.45
1:B:142:ARG:O	1:B:146:MET:HG3	2.16	0.45
1:B:286:LEU:HD22	1:B:297:VAL:HG21	1.97	0.45
1:A:406:VAL:HG13	1:A:417:LYS:HD3	1.99	0.45
1:A:185:ILE:HG13	1:A:404:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:TYR:HA	1:B:300:VAL:HG12	1.98	0.44
1:A:258:VAL:O	1:A:262:GLU:HG3	2.18	0.43
1:A:474:ILE:O	1:A:477:MET:N	2.52	0.43
1:B:250:LYS:HE2	1:B:250:LYS:HB3	1.69	0.42
1:A:145:MET:HG2	1:A:533:ALA:HB1	2.01	0.42
1:B:311:ASN:HB3	1:B:393:ARG:CZ	2.49	0.42
1:B:162:VAL:HG12	1:B:168:ILE:HG13	2.02	0.41
1:A:246:LEU:HD23	1:A:274:VAL:HB	2.03	0.41
1:B:365:ALA:O	1:B:369:LYS:HG3	2.20	0.41
1:B:448:ILE:N	1:B:449:PRO:HD2	2.36	0.41
1:B:369:LYS:O	1:B:373:GLU:HG3	2.19	0.41
1:B:251:ILE:HG21	1:B:257:ILE:HD13	2.02	0.41
1:A:257:ILE:H	1:A:257:ILE:HG13	1.80	0.40
1:A:151:VAL:HG21	1:A:472:LEU:HD11	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	382/586 (65%)	372 (97%)	10 (3%)	0	100	100
1	B	382/586 (65%)	375 (98%)	7 (2%)	0	100	100
All	All	764/1172 (65%)	747 (98%)	17 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	302/462 (65%)	289 (96%)	13 (4%)	29	35
1	B	304/462 (66%)	293 (96%)	11 (4%)	35	43
All	All	606/924 (66%)	582 (96%)	24 (4%)	31	39

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	ARG
1	A	163	THR
1	A	209	ASP
1	A	221	ARG
1	A	223	TYR
1	A	258	VAL
1	A	290	ARG
1	A	292	LYS
1	A	314	ARG
1	A	380	ASN
1	A	382	THR
1	A	452	ASP
1	A	458	ASN
1	B	157	ASN
1	B	217	MET
1	B	220	ASP
1	B	223	TYR
1	B	266	GLN
1	B	284	SER
1	B	290	ARG
1	B	314	ARG
1	B	416	GLU
1	B	458	ASN
1	B	520	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	458	ASN
1	B	157	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	386/586 (65%)	0.41	33 (8%)	10 16	35, 65, 107, 151	0
1	B	386/586 (65%)	0.35	23 (5%)	21 32	36, 70, 105, 137	0
All	All	772/1172 (65%)	0.38	56 (7%)	15 22	35, 67, 107, 151	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	382	THR	4.9
1	A	385	TYR	4.4
1	A	477	MET	4.2
1	A	514	VAL	4.2
1	A	381	THR	4.2
1	A	476	ALA	4.0
1	B	382	THR	3.7
1	A	117	THR	3.6
1	A	378	LEU	3.5
1	A	298	VAL	3.4
1	A	387	LYS	3.2
1	B	164	THR	3.1
1	A	384	ASP	3.0
1	A	297	VAL	3.0
1	B	297	VAL	3.0
1	A	517	GLY	3.0
1	B	274	VAL	3.0
1	A	478	THR	3.0
1	B	412	VAL	2.9
1	A	272	VAL	2.9
1	A	479	ILE	2.9
1	A	455	GLN	2.8
1	B	163	THR	2.8
1	A	121	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	273	ILE	2.8
1	B	477	MET	2.7
1	B	478	THR	2.7
1	B	299	ALA	2.7
1	A	274	VAL	2.6
1	A	273	ILE	2.5
1	A	452	ASP	2.5
1	A	516	LYS	2.5
1	A	515	GLU	2.5
1	B	158	LEU	2.5
1	B	298	VAL	2.5
1	A	329	ALA	2.5
1	A	275	ALA	2.4
1	B	195	ARG	2.4
1	B	268	ARG	2.4
1	A	278	VAL	2.4
1	A	397	LEU	2.4
1	B	203	ASP	2.4
1	A	475	PRO	2.3
1	B	479	ILE	2.3
1	A	271	LEU	2.3
1	A	513	MET	2.3
1	B	300	VAL	2.3
1	B	272	VAL	2.2
1	A	299	ALA	2.2
1	B	452	ASP	2.2
1	A	286	LEU	2.2
1	B	161	PRO	2.1
1	B	411	ASP	2.1
1	B	456	THR	2.1
1	B	348	VAL	2.0
1	A	154	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.